1,2-Cyclohexanedicarboxylic acid, 3-methylbut-2-yl pentyl ester

Inchi: InChI=1S/C18H32O4/c1-5-6-9-12-21-17(19)15-10-7-8-11-16(15)18(20)22-14(4)13(2)3/h1

InchiKey: DDTQSZRDTBBZJM-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-355.30	kJ/mol	Joback Method
hf	-881.03	kJ/mol	Joback Method
hfus	33.81	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.114		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	777.82	K	Joback Method
tc	976.97	K	Joback Method
tf	410.08	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.75	J/mol×K	777.82	Joback Method
cpg	869.25	J/mol×K	811.01	Joback Method
cpg	887.45	J/mol×K	844.20	Joback Method
cpg	904.36	J/mol×K	877.39	Joback Method
cpg	919.99	J/mol×K	910.59	Joback Method
cpg	934.35	J/mol×K	943.78	Joback Method
cpg	947.45	J/mol×K	976.97	Joback Method
dvisc	0.0017505	Pa×s	410.08	Joback Method

dvisc	0.0007450	Pa×s	471.37	Joback Method
dvisc	0.0003860	Pa×s	532.66	Joback Method
dvisc	0.0002290	Pa×s	593.95	Joback Method
dvisc	0.0001498	Pa×s	655.24	Joback Method
dvisc	0.0001054	Pa×s	716.53	Joback Method
dvisc	0.0000784	Pa×s	777.82	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339558&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume